

# Chapter 3.5: Classical degrees of freedom

*6N continuous variables*

classical microstate  $\{\vec{r}_1, \vec{p}_1, \vec{r}_2, \vec{p}_2, \vec{r}_3, \vec{p}_3, \dots, \vec{r}_N, \vec{p}_N\}$ , phase space integration:  $\prod_j d^3\vec{r}_j d^3\vec{p}_j = d\Gamma^{6N}$  (x  $\frac{1}{h^3}$ )

More general:  $\{q_1, q_2, q_3, q_4, \dots\}$  with energy  $\varepsilon(q_1, q_2, q_3, q_4, \dots)$  (not necessarily independent)

Integration:  $d\Gamma = \prod_j dq_j$  (x  $\frac{1}{h^3}$ )

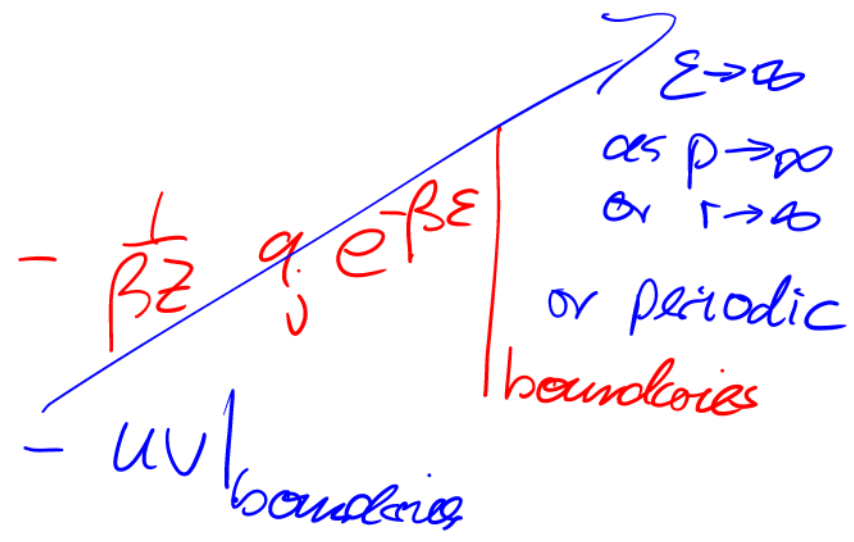
*general canonical degrees of freedom which are continuous*

Consider:  $\left\langle q_j \frac{\partial \varepsilon}{\partial q_k} \right\rangle = \frac{1}{Z} \int d\Gamma q_j \frac{\partial \varepsilon}{\partial q_k} e^{-\beta \varepsilon} = -\frac{1}{\beta Z} \int d\Gamma q_j \frac{\partial e^{-\beta \varepsilon}}{\partial q_k}$

*u v'*

$$= +\frac{1}{\beta Z} \int d\Gamma \frac{\partial q_j}{\partial q_k} e^{-\beta \varepsilon}$$

$$= \frac{1}{\beta} \left\langle \frac{\partial q_j}{\partial q_k} \right\rangle = \underline{k_B T} \quad -u' \quad v$$



**Def. 3.4:** The virial theorem for statistical mechanics states, that for continuous classical variables

$$\left\langle q_j \frac{\partial \varepsilon}{\partial q_k} \right\rangle = \delta_{jk} k_B T$$

prerequisite:  $\Sigma \rightarrow \infty$  at "boundaries"

or  $q_j$  periodic

3.5-3 Classical degrees of freedom

Special case: Bilinear energy  $\varepsilon = \sum_{jk} A_{jk} q_j q_k = \sum_j \varepsilon_j$  where  $\varepsilon_j = q_j \sum_k A_{jk} q_k$

$A_{jk} = A_{kj}$  (double counting)

$$\frac{\partial \varepsilon}{\partial q_l} = \sum_{j \neq k} \left( A_{jk} \frac{\partial q_j}{\partial q_l} q_k + A_{jk} q_j \frac{\partial q_k}{\partial q_l} \right) + \sum_j A_{jj} \frac{\partial q_j^2}{\partial q_l}$$

$$\frac{\partial q_j}{\partial q_l} = \delta_{jl}$$

$$= 2 \sum_k A_{lk} q_k$$

$$\varepsilon_j = q_j \sum_k A_{jk} q_k = \frac{1}{2} q_j \frac{\partial \varepsilon}{\partial q_j}$$

**Def. 3.5:** The equipartition theorem for statistical mechanics states, that for an classical energy

$$\varepsilon = \sum_j \varepsilon_j \text{ with } \varepsilon_j = \sum_k A_{jk} q_j q_k$$

also possible by using change of variables

or by solving for eigenmodes (diagonal form of  $A_{jk}$ )

$$\langle \varepsilon_j \rangle = \frac{1}{2} k_B T = \frac{1}{2} \langle q_j \frac{\partial \varepsilon}{\partial q_j} \rangle \text{ Virial}$$

$$C = \frac{\partial \langle \varepsilon_j \rangle}{\partial T} = \frac{1}{2} k_B$$

ideal gas  $\varepsilon = \sum_j \frac{p_j^2}{2m}$  3N momenta

$$E = \langle \varepsilon \rangle = \frac{3}{2} N \cdot k_B T$$